Lanford on StatMech, Jan 6 2010

January-06-10
10:01 AM

Class URL: http://www.math.ethz.ch/~lanford/Toronto/

Content:

- Microcanonical entropy (aka "large deviations")
- Gibbs states

In the context of classical lattice systems.

Statistical mechanics: Reconciling two different views of the physical world:

- Atomic physics: macroscopic matter is made up of very many small particles in constant motion.
- A glass of water left to itself can be described by just two parameters — temperature & pressure.

Recipe: The Boltzmann-Gibbs prescription permits in principle the calculation of bulk properties of macroscopic matter from the basic physics of the molecules making it up.

The justification of this recipe is one of the main goals of this course.

[Though in practice, calculating real quantities such as the boiling temp. of water is totally out of reach]

Orders of Magnitude:

A gram mole of some substance is a quantity whose

A gram mole of some substance is a quantity whose mass in grams is equal to the molecular weight of the substance [For water ~ 18]. This is the "Avogadro number" of molecules

$$\text{"} = 6.022 \times 10^{23}$$

So a glass of water has about $6 \cdot 10^{24} \times H_2O$.

$$\text{Vol per molecule} \simeq \frac{18}{6 \cdot 10^{23}} \simeq (3 \times 10^{-8})^3$$

size of H_2O $\simeq$ distance between molecules

Speed of sound $\approx 600\,m/s$

Time to travel distance between molecules: 5×10^{-13} sec

$\sim$ time between collisions of water molecules.

Water vapor is about 1,000 times less dense than water, so time between collisions $\sim 5 \times 10^{-12}$ sec.

~~Hamiltonian Dynamics:~~

N point particles moving in $\mathbb{R}^d$ $(d \sim 3)$

$\vec{q}_i$ position of i'th particle

$\vec{F}_i$ Force on ith particle, depends only on $\{q_j\}$

Newton's eqn:

$$m_i \frac{d^2 \vec{q}_i}{dt^2} = \vec{F}_i(\vec{q}_1 \dots \vec{q}_N)$$

Assume $F_i = -\text{grad}_{q_i} U(\vec{q}_1 \dots \vec{q}_n)$

Let $\vec{p}_i := m_i \dot{\vec{q}}_i$ & get

$$\frac{dq_i}{dt} = \frac{p_i}{m}, \quad \frac{dp_i}{dt} = -\text{grad}_{q_i}(U)$$

Let $T(p_1 \ldots p_N) = \sum \frac{1}{2m_i}|p_i|^2$ "the kinetic energy"

& $H := T + U$

Get

$$\frac{dq_i}{dt} = +\mathrm{grad}_{p_i} H \qquad \frac{dp_i}{dt} = -\mathrm{grad}_{q_i} H$$

Ignoring the grouping into triples, we get

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p} \qquad \frac{dp_i}{\partial t} = -\frac{\partial H}{\partial q_i}$$

.... H is a conserved quantity.
$\underset{\text{"energy"}}{\overset{}{\parallel}}$

..... Euclidean volume is preserved.

... the symplectic form $\omega = \sum dq_i \wedge dp_i$ is preserved. $(\mathrm{vol} = \omega^m$, where $m = d \cdot N)$

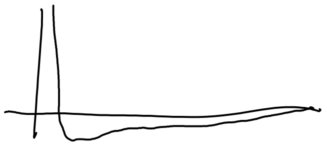
We want to constrain the particles to stay in some bounded region Λ, "the box".

$\longrightarrow$ Add to the interaction energy a term corresponding to the walls of the box:

$U = U_{wall} + U_{interparticle}$, where (2-body interaction)

$$U_{interparticle} = \sum_{i<j} \Phi(\vec{q}_i, \vec{q}_j)$$

often $\Phi(q_1, q_2) = \phi(|q_1 - q_2|)$ where

ϕ looks like 

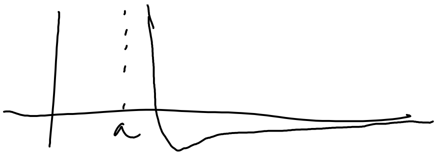
$\phi(r) \xrightarrow[r \to 0]{} \infty$

$\phi(r) \xrightarrow[r \to \infty]{} 0$ (rapidly)

So particles repel each other when they come close.)

Sometimes

Sometimes



Typically we want $\phi(q)$ to be integrable at ∞ so we exclude Columb.

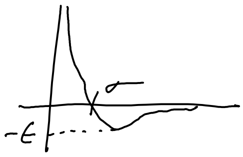
often we just restrict to finite range.

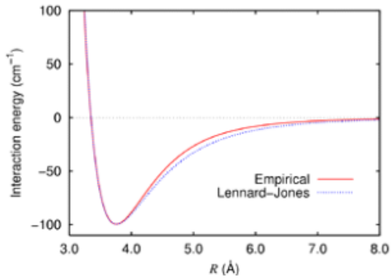
More properties: $\phi'(r) > 0$ for large r

(so particles that are far apart attract each other)

Example: The Lennard-Jones potential,

$$\phi(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$





Pasted from <http://en.wikipedia.org/wiki/Lennard-Jones_potential>